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Supporting Information

Metal–Porphyrin (M=Ti, Fe, Co, Ni, Cu, or Zn), A Potential Catalyst for the Oxidation of CO by N_2O: Insight from DFT Calculations

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Contents

1. Adsorption of the N_2O and CO on metal-porphyrin

Table S1. Adsorption energy of the N_2O and CO on metal-porphyrin.

	Ti-Pro	Fe-Pro	Co-Pro	Ni-Pro	Cu-Pro	Zn-Pro
M-CO	-33.6	-7.6	-10.5	-3.2	-3.2	-4.5
M-OC	-12.3	-2.9	-2.9	-3.2	-2.3	-2.5
M-ON$_2$	-8.8	-2.0	-1.9	-1.5	-0.6	-0.3
M-CO-ON$_2$	-36.5	-11.3	/	/	/	/
M-OC-ON$_2$	-2.7	7.3	/	/	/	/

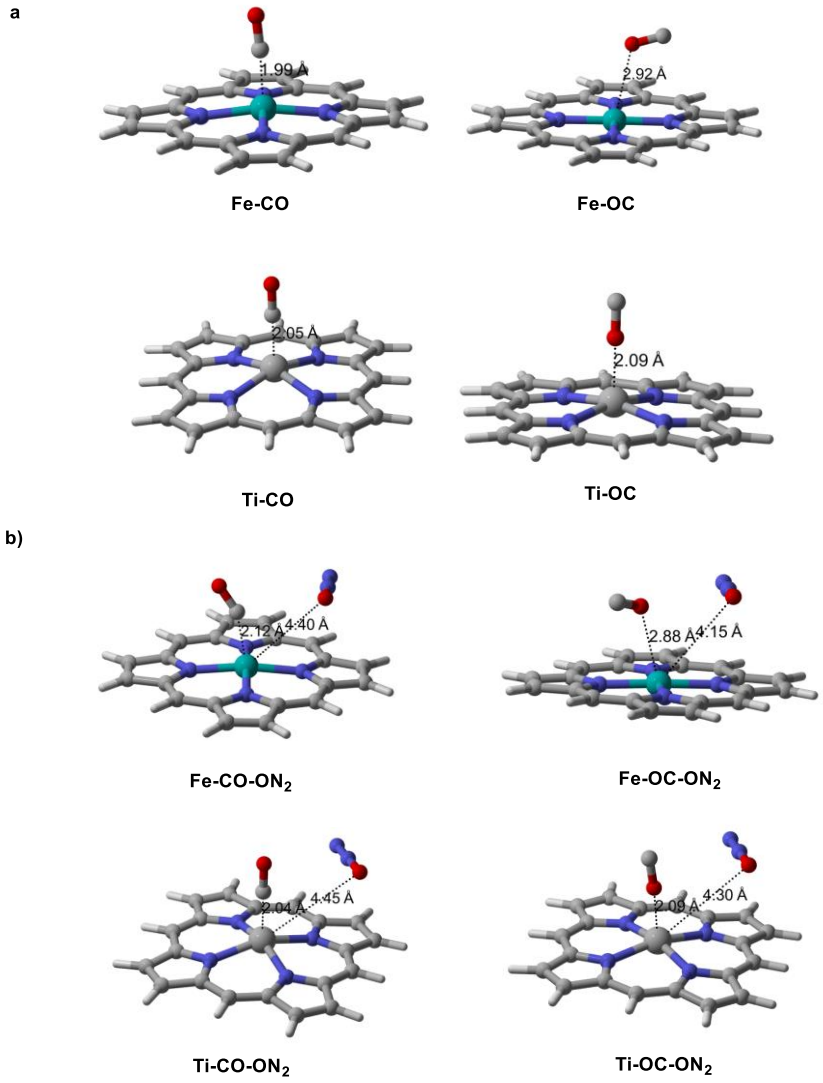

Figure S1. Optimized structures of the adsorption complexes of the reactant molecules: a) CO on Ti or Fe-porphyrin; b) coadsorption of CO and N_2O on Ti or Fe-porphyrin.

2. N_2O decomposition catalyzed by metal-porphyrin

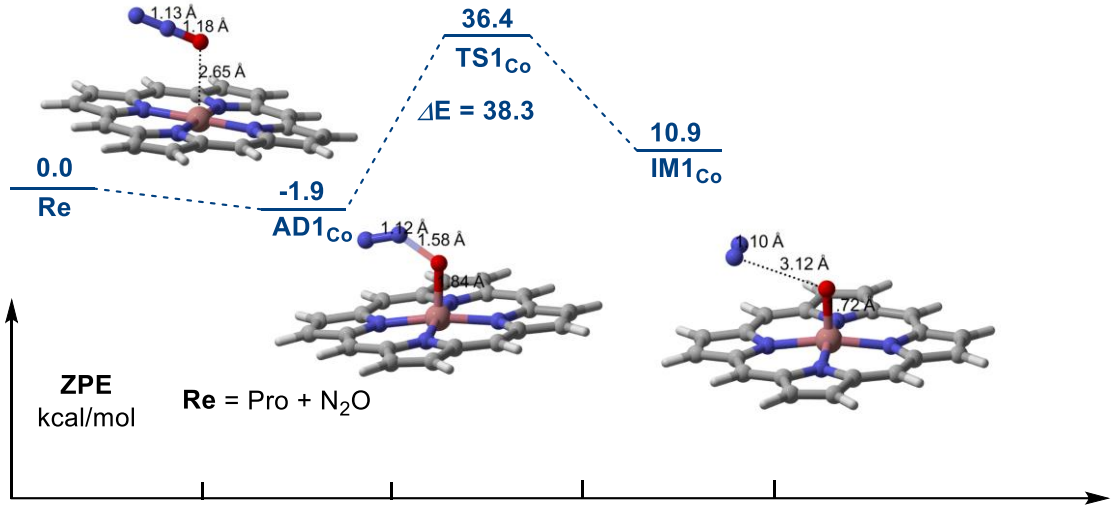

Figure S2. N_2O decomposition catalyzed by Co-porphyrin

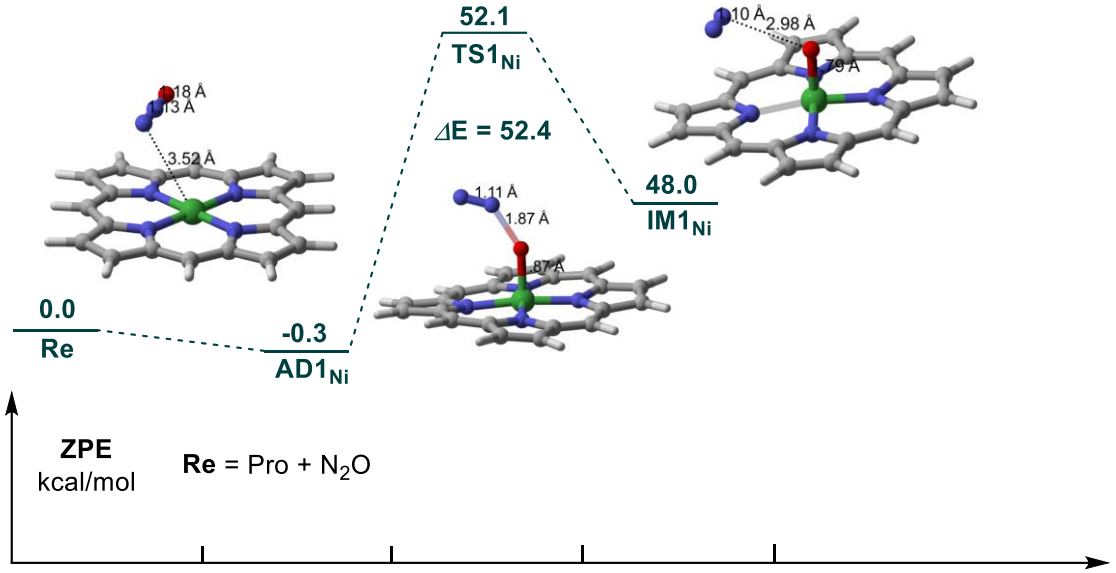

Figure S3. N_2O decomposition catalyzed by Ni-porphyrin

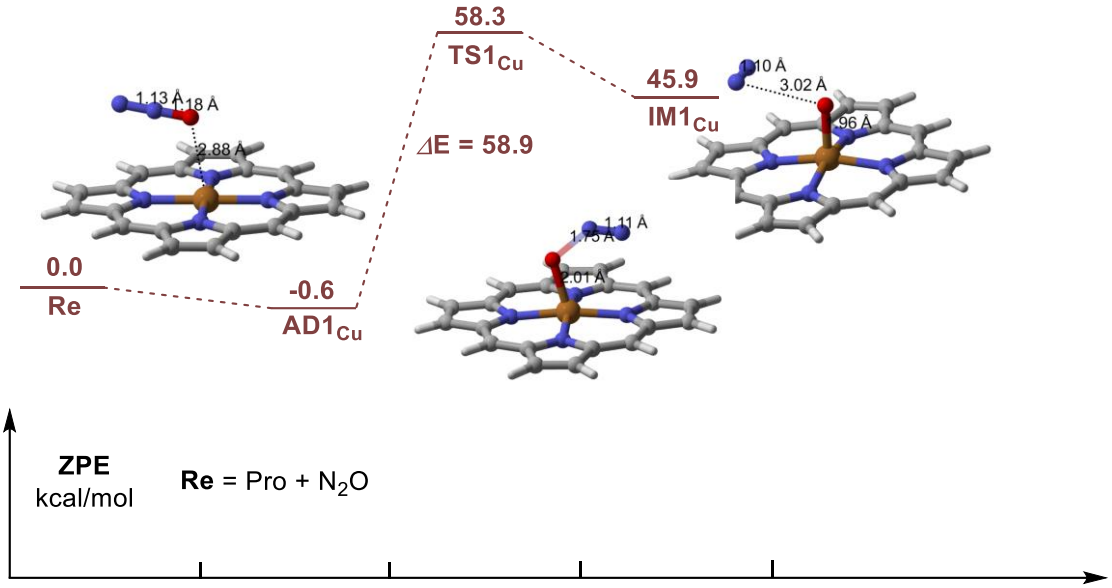

Figure S4. N_2O decomposition catalyzed by Cu-porphyrin

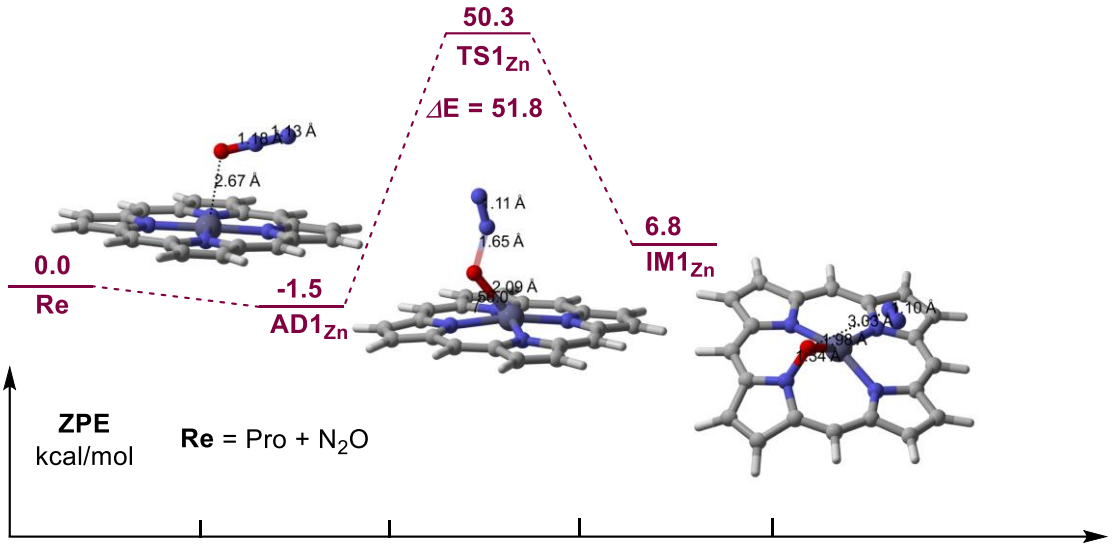

Figure S5. N_2O decomposition catalyzed by Zn-porphyrin

3. Bond length of N_2O decomposition and CO oxidation

Table S2. Bond length of TS for N_2O decomposition on metal-porphyrins.

	M-O / Å	O-N / Å	N-N / Å
Ti−porphyrin	2.02	1.25	1.14
Fe−porphyrin	1.86	1.48	1.13
Co−porphyrin	1.84	1.58	1.12
Ni−porphyrin	1.87	1.87	1.11
Cu−porphyrin	2.01	1.75	1.11
Zn−porphyrin	2.09	1.65	1.11

Table S3. Bond length of TS for CO oxidation by O-M-porphyrins.

	M-O / Å	O-C / Å	C-O / Å
O-Ti−porphyrin	1.62	1.77	1.15
O-Fe−porphyrin	1.62	1.75	1.15

4. Charge of N_2O decomposition and CO oxidation

Table S4. Charge of N_2O decomposition.

	M	O	N1	N2
Ti−porphyrin $_R$	1.22	-0.45	0.58	-0.02
Ti−porphyrin $_{TS}$	1.29	-0.42	0.43	-0.20
Fe−porphyrin $_R$	0.45	-0.46	0.58	-0.09
Fe−porphyrin $_{TS}$	0.40	-0.34	0.18	-0.18
Co−porphyrin $_R$	0.35	-0.45	0.57	-0.09
Co−porphyrin $_{TS}$	0.30	-0.30	0.15	-0.12
Ni−porphyrin $_R$	0.25	-0.45	0.57	-0.12
Ni−porphyrin $_{TS}$	0.26	-0.44	0.10	-0.11
Cu−porphyrin $_R$	0.11	-0.45	0.57	-0.11

Cu−porphyrin $_{TS}$	0.13	-0.34	0.13	-0.08
Zn−porphyrin $_{R}$	0.47	-0.45	0.59	-0.10
Zn−porphyrin $_{TS}$	0.52	-0.34	0.19	-0.09

Table S5. Charge of CO oxidation.

	M	O1	C	O2
O-Ti−porphyrin $_{R}$	1.29	-0.56	0.12	-0.15
O-Ti−porphyrin $_{TS}$	1.21	-0.50	0.23	-0.25
O-Fe−porphyrin $_{R}$	0.45	-0.41	0.79	-0.36
O-Fe−porphyrin $_{TS}$	0.44	-0.39	0.20	-0.29

Table S6. Charge difference of N_2O or CO between transition state and adsorbed complex.

	Ti−porphyrin	Fe−porphyrin	O-Fe−porphyrin	O-Fe−porphyrin
q_{diff}	-0.30	-0.37	-0.52	0.01

5. Oxidation of CO by N_2O on O-Ti-porphyrin

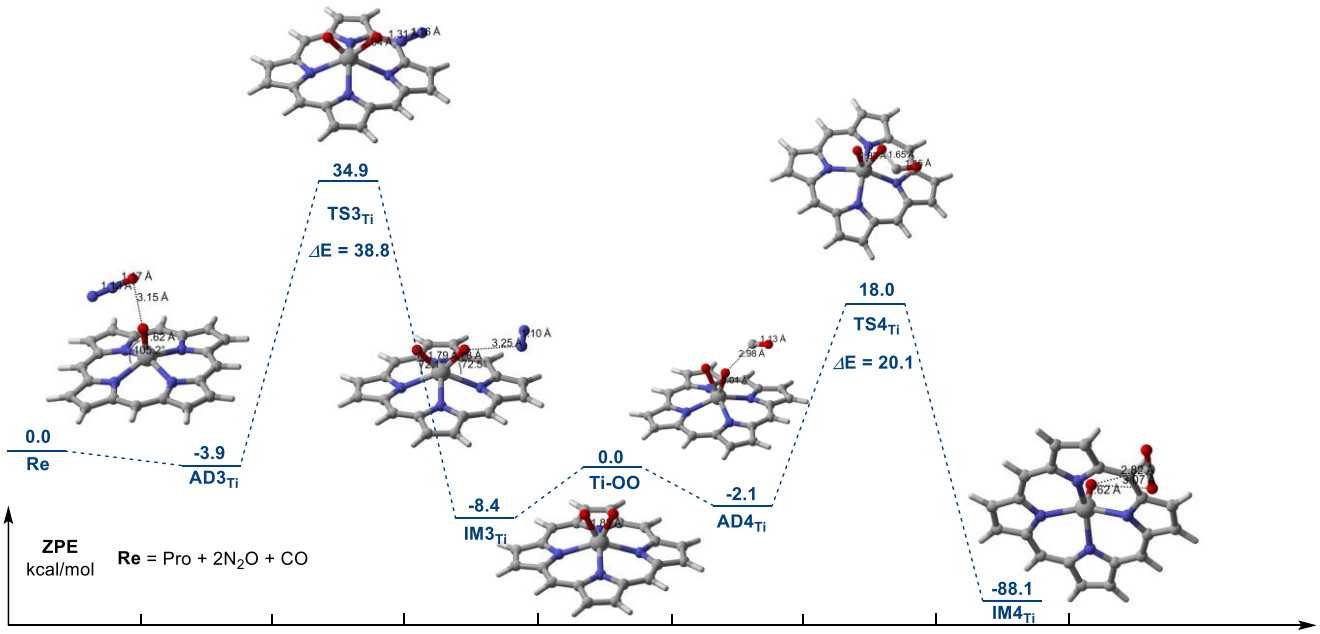

Figure S6. N_2O decomposition and oxidation of CO on O-Ti-porphyrin

6. Oxidation of CO by N_2O on O-Fe-porphyrin

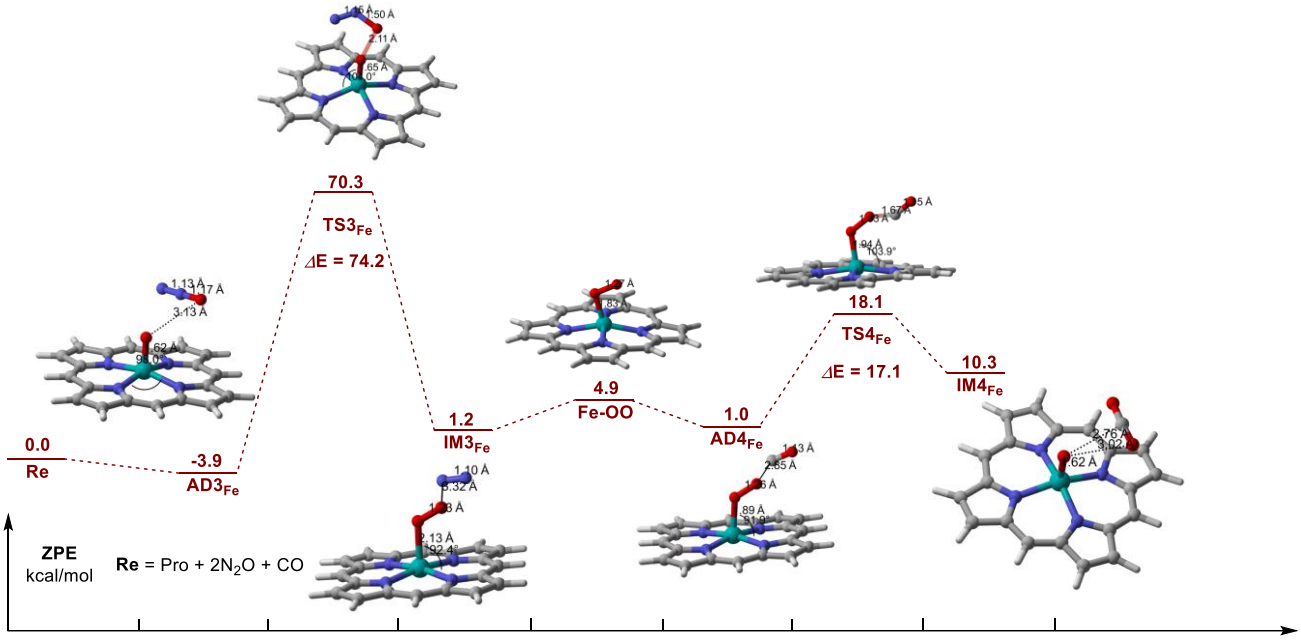

Figure S7. N_2O decomposition and oxidation of CO on O-Fe-porphyrin

7. Cartesian coordinates of all transition states

$TS1_{Ti}$

0 3

N	-0.15557400	2.04922300	-0.28838500
N	-2.19113500	0.00001100	-0.10588200
N	-0.15562100	-2.04923000	-0.28828500
N	1.88576900	-0.00005000	-0.54715100
Ti	-0.11047600	0.00001800	-0.00215400
O	0.42197600	0.00010900	1.94648300
N	1.47633100	0.00006100	2.62127100
N	2.02816900	-0.00002000	3.62384100
C	-0.84337800	4.24231800	-0.36718900
C	0.51281900	4.24074500	-0.49195100
C	0.94513300	2.87250700	-0.45362300
C	-1.26387000	2.87532100	-0.24690000
C	-4.37747800	-0.68459400	-0.01340400
C	-4.37745800	0.68468100	-0.01339200
C	-3.01666000	1.10793200	-0.07761700
C	-3.01669200	-1.10788200	-0.07762900
C	0.51271500	-4.24076800	-0.49193300
C	-0.84348300	-4.24231000	-0.36719100
C	-1.26394100	-2.87530400	-0.24686300
C	0.94506100	-2.87254400	-0.45355400
C	4.05905700	0.68495200	-0.78378200
C	4.05904600	-0.68508400	-0.78377600
C	2.70545000	-1.10853500	-0.63089600
C	2.70546800	1.10842600	-0.63090900

C	-2.57486400	-2.43317100	-0.13118900
C	2.25583500	-2.43250300	-0.58275000
C	2.25589300	2.43241100	-0.58279900
C	-2.57479800	2.43321400	-0.13119000
H	4.90722300	-1.35082900	-0.88012300
H	4.90724400	1.35068300	-0.88014200
H	1.17268400	5.09014200	-0.61511600
H	-1.51252600	5.09336400	-0.36803100
H	-5.22991100	1.35123900	0.01757500
H	-5.22994900	-1.35113100	0.01755300
H	-1.51265200	-5.09333800	-0.36808000
H	1.17256200	-5.09017500	-0.61512100
H	3.01580900	-3.20215800	-0.68629200
H	-3.34515300	3.19909100	-0.10849200
H	-3.34523600	-3.19903100	-0.10852100
H	3.01589700	3.20203700	-0.68633000

$TS2_{Ti}$

0 3

N	-1.25694300	-1.41013500	-0.54527000
N	1.59995400	-1.45447700	-0.14222400
N	1.66367600	1.40312500	-0.14393500
N	-1.17783800	1.49163800	-0.51082200
Ti	0.09596600	-0.00767500	0.19939700
O	-0.49990800	-0.09016000	1.82396900
C	-2.17187800	-0.24701200	2.39464800
O	-2.37074800	0.16956800	3.44610900
C	-2.35097500	-3.41474500	-0.77425500

C	-3.29871400	-2.42261400	-0.76925600
C	-2.60091400	-1.18786000	-0.62339700
C	-1.08665900	-2.78368500	-0.61465600
C	3.60585900	-2.58405800	-0.02001900
C	2.62435200	-3.51742400	-0.16787500
C	1.38103800	-2.81259600	-0.25236400
C	2.96481600	-1.30038100	-0.01020200
C	2.77368100	3.41586700	-0.11537400
C	3.71048800	2.42549900	0.05167700
C	3.00837800	1.18874500	0.02439000
C	1.51201400	2.77551900	-0.23781600
C	-3.17820600	2.59934600	-0.77165600
C	-2.19079300	3.53830800	-0.78972700
C	-0.94944400	2.84850100	-0.60837400
C	-2.54068200	1.32302400	-0.60929400
C	3.61266100	-0.08212500	0.10499200
C	0.29847700	3.43355000	-0.46511800
C	-3.19336000	0.09541600	-0.60183800
C	0.14432700	-3.41573700	-0.47303100
H	-2.29004700	4.61059700	-0.90066500
H	-4.24535900	2.74665000	-0.87468900
H	-4.37296800	-2.52247200	-0.85140200
H	-2.50404800	-4.48343500	-0.85194000
H	2.72760300	-4.59313900	-0.23335900
H	4.67407200	-2.73977400	0.05749200
H	4.78270400	2.52781100	0.15619500
H	2.93294600	4.48531900	-0.16834200
H	0.34231700	4.51760700	-0.53223200

H	0.14497800	-4.50032400	-0.54627200
H	4.69052300	-0.10351700	0.23628700
H	-4.27746700	0.12396200	-0.67139400

$TS3_{Ti}$

0 3

N	-2.26148500	-0.05625700	-0.32907300
N	-0.16988600	-2.01192500	-0.16433900
N	1.75822000	0.07534700	-0.70797500
N	-0.28258400	2.02820200	-0.12726200
Ti	-0.21645800	-0.00127200	0.61402900
O	-1.18770200	0.01836900	1.94851500
O	1.31597200	-0.07613000	1.96124500
N	2.59102400	-0.35835300	1.92164200
N	3.59920200	0.21266200	1.97453100
C	-4.44551700	-0.80314500	-0.31690600
C	-4.48496000	0.55619200	-0.30687300
C	-3.11808800	1.00635800	-0.28436500
C	-3.05697900	-1.17442300	-0.30115400
C	0.57777000	-4.17323800	-0.40892200
C	-0.78149100	-4.22654900	-0.27870200
C	-1.23282400	-2.87574000	-0.15844000
C	0.94157500	-2.78883100	-0.37282200
C	3.89339900	0.82482300	-1.18424300
C	3.92362300	-0.53428900	-1.23353300
C	2.59549500	-0.97901900	-0.89779300
C	2.54641100	1.18612700	-0.82814500
C	-1.03959800	4.19936000	-0.24407800
C	0.32028700	4.23569100	-0.36687100

C	0.77462700	2.87950400	-0.32792700
C	-1.40083500	2.81935300	-0.12843000
C	2.22050000	-2.30823300	-0.67713900
C	2.08636400	2.48325200	-0.60862200
C	-2.71262300	2.33629200	-0.17458000
C	-2.57363300	-2.47297700	-0.19791500
H	0.95805500	5.09816800	-0.51118700
H	-1.73895800	5.02456800	-0.27313000
H	-5.35246700	1.20326200	-0.30077000
H	-5.27427800	-1.49929900	-0.32217500
H	-1.42385300	-5.09708600	-0.30647900
H	1.26900800	-4.99082400	-0.56678800
H	4.76537700	-1.18013100	-1.44697600
H	4.70441800	1.52150100	-1.35202100
H	2.81184400	3.28479700	-0.72866100
H	-3.31567300	-3.26812800	-0.18474200
H	2.99146100	-3.06231300	-0.81795300
H	-3.50147200	3.08478900	-0.16371500

TS4$_{Ti}$

0 3

N	1.73069500	0.56941900	-0.61946000
N	-0.75051200	1.94993400	-0.28142900
N	-2.13541800	-0.59613300	-0.21574700
N	0.41522000	-1.94108000	-0.37395900
Ti	-0.17553300	-0.00471700	0.21463000
O	0.60091800	0.50662700	2.15345800
O	-0.61191800	-0.16440100	2.07907400
C	1.94268900	-0.44107300	2.32265400

O	2.93962000	0.09963000	2.52369300
C	3.61766400	1.85769100	-0.91040500
C	4.00393000	0.55265800	-0.99340900
C	2.82781500	-0.24047400	-0.80351100
C	2.20491400	1.86105700	-0.68047400
C	-2.05232300	3.84749500	-0.28865700
C	-0.75662100	4.24708300	-0.42132900
C	0.04877700	3.06181600	-0.42400900
C	-2.04712000	2.41393800	-0.21838400
C	-4.04039200	-1.87611200	-0.18400400
C	-4.43009600	-0.56588400	-0.16239200
C	-3.23844000	0.22482200	-0.17645700
C	-2.61158100	-1.88602600	-0.21058800
C	1.65886700	-3.86046100	-0.65917200
C	0.36500800	-4.24227200	-0.47379900
C	-0.41225500	-3.04604400	-0.32273900
C	1.68352400	-2.42850600	-0.60702400
C	-3.18593000	1.61803400	-0.15834600
C	-1.79898900	-3.01736900	-0.23112800
C	2.80547600	-1.63442200	-0.79003800
C	1.42660100	3.01339100	-0.57455000
H	-0.04276700	-5.24521000	-0.46620200
H	2.52408600	-4.48664000	-0.83550100
H	4.99443500	0.15517400	-1.17382900
H	4.22791900	2.74598100	-1.01351900
H	-0.37389000	5.25481800	-0.52159800
H	-2.94289000	4.46224200	-0.25785900
H	-5.43652400	-0.16831700	-0.13357500

H	-4.66620500	-2.75944600	-0.17552400
H	-2.30245800	-3.98033000	-0.22132200
H	1.94843300	3.96294300	-0.65531400
H	-4.13885500	2.13938000	-0.12951300
H	3.75248600	-2.14269900	-0.94716000

$TS1_{Fe}$

0 3

N	-0.12821200	1.99795500	-0.31812000
N	-2.11731800	0.00084600	-0.13982600
N	-0.12991200	-1.99794200	-0.31801100
N	1.86090700	-0.00083400	-0.39622200
Fe	-0.11067400	-0.00000800	-0.07102000
O	-0.04661400	-0.00002900	1.78893800
N	1.14221500	0.00003000	2.66474200
N	2.26467300	-0.00009900	2.49738100
C	-0.80776300	4.20084700	-0.29224200
C	0.54965400	4.20065400	-0.38183100
C	0.96221800	2.82995400	-0.38897700
C	-1.21843500	2.83035300	-0.24501600
C	-4.31770400	-0.67799900	-0.01150700
C	-4.31710800	0.68159300	-0.01138300
C	-2.94799000	1.09394700	-0.09260000
C	-2.94894500	-1.09153900	-0.09277400
C	0.54609300	-4.20122100	-0.38143800
C	-0.81134800	-4.20025200	-0.29220200
C	-1.22086000	-2.82940900	-0.24512000
C	0.95983000	-2.83087300	-0.38857500
C	4.06000800	0.67798100	-0.58147600

C	4.05944000	-0.68155300	-0.58125800
C	2.69462900	-1.09497700	-0.46537100
C	2.69554500	1.09258900	-0.46569400
C	-2.53589000	-2.41141300	-0.13619300
C	2.27854900	-2.41395700	-0.45318300
C	2.28057400	2.41192200	-0.45374400
C	-2.53380500	2.41346900	-0.13589800
H	4.90078400	-1.35845900	-0.65410600
H	4.90191900	1.35415800	-0.65454300
H	1.22442100	5.04527100	-0.43573600
H	-1.48335200	5.04581800	-0.25709600
H	-5.16015100	1.35893000	0.03397400
H	-5.16134100	-1.35460300	0.03373600
H	-1.48766700	-5.04464300	-0.25719300
H	1.22015100	-5.04641600	-0.43514500
H	3.04485600	-3.18128600	-0.50717700
H	-3.30029400	3.18104200	-0.08699500
H	-3.30304000	-3.17833600	-0.08744400
H	3.04751800	3.17859700	-0.50798300

$TS2_{Fe}$

0 3

N	0.14549000	-1.99130100	-0.31588900
N	2.12899200	0.00060400	-0.15311600
N	0.14428700	1.99132500	-0.31599700
N	-1.83979600	-0.00065100	-0.45176200
Fe	0.12256200	-0.00005100	-0.02749000
O	0.01167800	0.00011400	1.65984200

C	-1.26104100	-0.00005000	2.86303800
O	-2.35115800	0.00021300	2.48960100
C	0.82390900	-4.19638700	-0.26924600
C	-0.53177800	-4.19643900	-0.37007600
C	-0.94384300	-2.82570100	-0.39018100
C	1.23411500	-2.82564400	-0.22767100
C	4.32853700	0.68089900	0.00272900
C	4.32897500	-0.67834600	0.00242300
C	2.96118100	-1.09097800	-0.08891200
C	2.96048200	1.09269700	-0.08848100
C	-0.53431300	4.19603000	-0.37067100
C	0.82134500	4.19682200	-0.26941400
C	1.23237400	2.82633000	-0.22756600
C	-0.94553400	2.82502500	-0.39068500
C	-4.03839500	-0.68069200	-0.63941200
C	-4.03879200	0.67808800	-0.63953000
C	-2.67398800	1.09094200	-0.51668300
C	-2.67334800	-1.09273000	-0.51651100
C	2.54674600	2.41166300	-0.11820300
C	-2.26151200	2.40939800	-0.48132000
C	-2.26007900	-2.41092300	-0.48081900
C	2.54826600	-2.41018000	-0.11873900
H	-4.87938400	1.35550500	-0.71548000
H	-4.87859200	-1.35860800	-0.71528400
H	-1.20701100	-5.04033600	-0.42769100
H	1.50022600	-5.04028700	-0.22604300
H	5.17131600	-1.35584500	0.05606800
H	5.17044300	1.35891300	0.05668400

H	1.49713500	5.04113900	-0.22612000
H	-1.21004100	5.03950700	-0.42861900
H	-3.02770400	3.17682200	-0.53468100
H	3.31400100	-3.17747600	-0.05676500
H	3.31199700	3.17942000	-0.05596200
H	-3.02579500	-3.17883400	-0.53398600

$TS3_{Fe}$

0 3

N	-0.77522600	1.98481700	-0.31510100
N	-2.23513800	-0.47687500	-0.14019200
N	0.19799000	-1.94731300	-0.51173900
N	1.65722900	0.51651400	-0.69433200
Fe	-0.21329400	0.01199200	0.07227100
O	0.03191600	-0.01898800	1.70434400
O	1.71898900	-1.15320000	2.25064500
N	2.79555600	-0.13121600	2.48014400
N	2.59783300	0.98312300	2.27566800
C	-1.96132600	3.95126900	-0.14802100
C	-0.65298500	4.28348600	-0.32250600
C	0.07859000	3.05243400	-0.42145600
C	-2.02733700	2.51750300	-0.13896900
C	-4.18678100	-1.67504600	0.09576700
C	-4.51602700	-0.35524500	0.14875500
C	-3.29322100	0.38299100	0.00770600
C	-2.76373300	-1.74101400	-0.07924200
C	1.38492300	-3.91169000	-0.68290800
C	0.07966000	-4.24665900	-0.49310700
C	-0.65125800	-3.01617700	-0.38042500

C	1.44934400	-2.47767900	-0.68524500
C	3.60445200	1.71429100	-0.97045200
C	3.93101500	0.39464900	-1.03248700
C	2.71284500	-0.34352100	-0.85260900
C	2.18787400	1.78095200	-0.75089700
C	-2.02394400	-2.91455200	-0.18402300
C	2.61100400	-1.73041700	-0.84564900
C	1.45177900	2.95227800	-0.62065900
C	-3.19046800	1.77031700	0.01075600
H	4.90621500	-0.04949200	-1.18506600
H	4.25747800	2.57281600	-1.05905200
H	-0.21341700	5.27069000	-0.38483300
H	-2.81274200	4.61065400	-0.03827500
H	-5.49619500	0.08795400	0.26963700
H	-4.84229100	-2.53377700	0.16395600
H	-0.35867600	-5.23460700	-0.43411800
H	2.23529100	-4.56913700	-0.81031300
H	3.53512700	-2.28740400	-0.97534800
H	-4.11480800	2.32739700	0.13923700
H	-2.57638600	-3.84738800	-0.10768100
H	2.00465800	3.88562700	-0.68419300

TS4$_{Fe}$

0 3

N	1.73069500	0.56941900	-0.61946000
N	-0.75051200	1.94993400	-0.28142900
N	-2.13541800	-0.59613300	-0.21574700
N	0.41522000	-1.94108000	-0.37395900
Ti	-0.17553300	-0.00471700	0.21463000

O	0.60091800	0.50662700	2.15345800
O	-0.61191800	-0.16440100	2.07907400
C	1.94268900	-0.44107300	2.32265400
O	2.93962000	0.09963000	2.52369300
C	3.61766400	1.85769100	-0.91040500
C	4.00393000	0.55265800	-0.99340900
C	2.82781500	-0.24047400	-0.80351100
C	2.20491400	1.86105700	-0.68047400
C	-2.05232300	3.84749500	-0.28865700
C	-0.75662100	4.24708300	-0.42132900
C	0.04877700	3.06181600	-0.42400900
C	-2.04712000	2.41393800	-0.21838400
C	-4.04039200	-1.87611200	-0.18400400
C	-4.43009600	-0.56588400	-0.16239200
C	-3.23844000	0.22482200	-0.17645700
C	-2.61158100	-1.88602600	-0.21058800
C	1.65886700	-3.86046100	-0.65917200
C	0.36500800	-4.24227200	-0.47379900
C	-0.41225500	-3.04604400	-0.32273900
C	1.68352400	-2.42850600	-0.60702400
C	-3.18593000	1.61803400	-0.15834600
C	-1.79898900	-3.01736900	-0.23112800
C	2.80547600	-1.63442200	-0.79003800
C	1.42660100	3.01339100	-0.57455000
H	-0.04276700	-5.24521000	-0.46620200
H	2.52408600	-4.48664000	-0.83550100
H	4.99443500	0.15517400	-1.17382900
H	4.22791900	2.74598100	-1.01351900

H	-0.37389000	5.25481800	-0.52159800
H	-2.94289000	4.46224200	-0.25785900
H	-5.43652400	-0.16831700	-0.13357500
H	-4.66620500	-2.75944600	-0.17552400
H	-2.30245800	-3.98033000	-0.22132200
H	1.94843300	3.96294300	-0.65531400
H	-4.13885500	2.13938000	-0.12951300
H	3.75248600	-2.14269900	-0.94716000

TS_{Co}

0 2

N	0.11214800	-1.98952400	-0.27327500
N	2.09761200	-0.00001200	-0.20344300
N	0.11217000	1.98952300	-0.27329400
N	-1.85814800	0.00000900	-0.41178400
Co	0.10558400	0.00000200	-0.14397900
O	0.20279900	0.00001300	1.69035000
N	-1.07866600	0.00000800	2.62140300
N	-2.18460800	-0.00000100	2.41597900
C	0.78952800	-4.19616100	-0.19033500
C	-0.56563300	-4.19776100	-0.27224800
C	-0.97541900	-2.82501900	-0.31831900
C	1.19961700	-2.82274000	-0.18747400
C	4.29968300	0.67911200	-0.07604500
C	4.29967900	-0.67915000	-0.07605100
C	2.92951500	-1.09075500	-0.14057200
C	2.92952300	1.09072400	-0.14056400
C	-0.56559900	4.19776300	-0.27224800
C	0.78956100	4.19615600	-0.19032100

C	1.19964500	2.82273000	-0.18746900
C	-0.97539100	2.82502500	-0.31833600
C	-4.06086000	-0.67926000	-0.58868500
C	-4.06085500	0.67929000	-0.58869400
C	-2.69691500	1.09253000	-0.47006600
C	-2.69692300	-1.09250400	-0.47005100
C	2.51627600	2.40906700	-0.12785300
C	-2.29027200	2.41110600	-0.41551400
C	-2.29029700	-2.41108400	-0.41549000
C	2.51625100	-2.40909400	-0.12787000
H	-4.90098300	1.35794900	-0.65866200
H	-4.90099000	-1.35791600	-0.65864100
H	-1.24379500	-5.04066300	-0.30441800
H	1.46826900	-5.03776500	-0.14039800
H	5.14103700	-1.35860300	-0.03307600
H	5.14104400	1.35856300	-0.03306500
H	1.46830400	5.03775700	-0.14036300
H	-1.24375900	5.04066700	-0.30441400
H	-3.05912800	3.17663800	-0.45541200
H	3.28285500	-3.17566300	-0.06772800
H	3.28288700	3.17562600	-0.06769600
H	-3.05916300	-3.17660600	-0.45538700

TS_{Ni}

0 1

N	-0.03144600	1.97115500	-0.38252300
N	-1.84438800	-0.15408900	-0.52457000
N	0.27904300	-1.95966400	-0.37378700

N	2.07548400	0.16314200	-0.19232300
Ni	0.12405800	0.00356300	-0.24936600
O	0.02259600	-0.01738700	1.62187400
N	-1.03238600	-0.04341600	3.16512000
N	-2.11405500	-0.07067800	3.39807000
C	-0.88256000	4.11322700	-0.47873300
C	0.44305000	4.22189500	-0.20739100
C	0.96086800	2.88888200	-0.14858000
C	-1.17328600	2.71344900	-0.55843700
C	-3.99274600	-0.99628600	-0.53306800
C	-4.08999400	0.34729700	-0.70048000
C	-2.75388600	0.86219700	-0.67022000
C	-2.59657100	-1.29700300	-0.42852000
C	1.12559000	-4.10521400	-0.34310100
C	-0.22671200	-4.20836600	-0.28765700
C	-0.74359000	-2.87355900	-0.30603200
C	1.42982500	-2.70669300	-0.36655400
C	4.19644800	1.00584700	0.13794400
C	4.32004300	-0.33654400	-0.02006100
C	2.99813700	-0.85389600	-0.20094200
C	2.80222100	1.30804900	0.02618700
C	-2.08947300	-2.57341100	-0.30370400
C	2.71001000	-2.19667200	-0.32023000
C	2.28842800	2.58622200	0.06823700
C	-2.44477200	2.20544500	-0.72451800
H	5.21456600	-0.94530200	-0.00475300
H	4.96803900	1.74649100	0.30254900
H	1.03866500	5.11419000	-0.06546400

H	-1.61998000	4.89600900	-0.59954200
H	-4.97642000	0.95694700	-0.81746400
H	-4.78125200	-1.73629700	-0.49173500
H	-0.84101100	-5.09842100	-0.24797900
H	1.86961700	-4.89099000	-0.34891800
H	3.53851000	-2.89739300	-0.31582100
H	-3.26075500	2.91070100	-0.84527000
H	-2.79309500	-3.39702800	-0.23847300
H	2.97678700	3.40609400	0.24536000

TS_{Cu}

0 2

N	1.92090600	-0.00596500	-0.39884500
N	-0.08881100	2.02640900	-0.35826400
N	-2.11342100	0.00667000	-0.21569700
N	-0.10164200	-2.02630600	-0.35847600
Cu	-0.09473300	-0.00051100	-0.15484300
O	-0.43355600	0.00027000	1.82236000
N	0.96301400	-0.00055700	2.87119500
N	2.05545200	-0.00202000	2.66512100
C	4.11913500	0.66710700	-0.50471900
C	4.11484700	-0.69323000	-0.50288400
C	2.74128400	-1.10346500	-0.43958400
C	2.74819900	1.08617600	-0.44225100
C	-0.75946100	4.22522000	-0.28612600
C	0.59820100	4.22168200	-0.36396900
C	1.00616800	2.84439900	-0.39459900
C	-1.17614400	2.85037000	-0.27040500

C	-4.30094200	-0.66674700	-0.01798300
C	-4.29657500	0.69367500	-0.01659700
C	-2.92648800	1.10543900	-0.13084900
C	-2.93350100	-1.08707500	-0.13289100
C	0.57166300	-4.22570000	-0.36103000
C	-0.78620500	-4.22070200	-0.28655400
C	-1.19435400	-2.84329300	-0.27237200
C	0.98836400	-2.85104200	-0.39169100
C	-2.49358000	2.42327700	-0.16737400
C	-2.50909200	-2.40766000	-0.17082500
C	2.30881100	-2.42262200	-0.43332600
C	2.32392400	2.40798600	-0.43798200
H	-1.46194100	-5.06513000	-0.23962200
H	1.24257100	-5.07484300	-0.38760500
H	4.95879400	-1.36974600	-0.54566100
H	4.96733400	1.33816900	-0.54925700
H	1.27440600	5.06654500	-0.39268400
H	-1.42982900	5.07385600	-0.23811200
H	-5.13894900	1.36994700	0.05284900
H	-5.14765300	-1.33772000	0.05010300
H	-3.27763600	-3.17264600	-0.10328500
H	3.09569500	3.17221200	-0.46745400
H	-3.25703600	3.19320500	-0.09834000
H	3.07595600	-3.19158000	-0.46054100

TS_{Zn}

0 1

N	0.12577000	2.04212400	-0.33450900

N	-1.95375100	-0.00757600	-0.42081600
N	0.13945200	-2.04263200	-0.33290600
N	2.19428900	0.00661300	-0.13135400
Zn	0.16178900	0.00014300	-0.08376100
O	-1.26429500	-0.00393100	1.44083400
N	-0.95427400	0.00261500	3.06027700
N	-1.31872700	0.01039000	4.10597800
C	-0.55753300	4.22935600	-0.45392300
C	0.80090700	4.23703900	-0.36146500
C	1.21953500	2.86083600	-0.28727600
C	-0.96957300	2.84884400	-0.43411600
C	-4.09926300	-0.70030000	-0.78670700
C	-4.10382300	0.67046300	-0.78748100
C	-2.76169300	1.10366200	-0.55627900
C	-2.75426700	-1.12426100	-0.55505000
C	0.82931700	-4.23310100	-0.35597200
C	-0.52912500	-4.23472300	-0.44828300
C	-0.95042900	-2.85696700	-0.43084900
C	1.23864800	-2.85398700	-0.28422700
C	4.37894600	0.69578600	-0.07425700
C	4.38353700	-0.66774400	-0.07362600
C	3.00846100	-1.08933500	-0.11882300
C	3.00106500	1.10806200	-0.11983100
C	-2.28046900	-2.43105100	-0.52895900
C	2.55857000	-2.41096100	-0.17767800
C	2.54237400	2.42663400	-0.18012400
C	-2.29667600	2.41368800	-0.53173800
H	5.23873400	-1.33174800	-0.05656000

H	5.22964600	1.36555900	-0.05775800
H	1.46553600	5.09184600	-0.34749900
H	-1.22708800	5.07703200	-0.53061400
H	-4.94697400	1.32680500	-0.96425000
H	-4.93801200	-1.36245900	-0.96273000
H	-1.19298900	-5.08700400	-0.52338800
H	1.49971800	-5.08336700	-0.34056100
H	3.32442000	-3.18250600	-0.15548300
H	-3.04866300	3.19234200	-0.63337200
H	-3.02715000	-3.21494700	-0.62942000
H	3.30311800	3.20324200	-0.15891000